STRUCTURE FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9 DICTIONARY FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CA roles and document type information have been removed from *

* the IDE default display format and the ED field has been added, *

* effective March 20, 2005. A new display format, IDERL, is now *

* available and contains the CA role and document type information. *

* *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10666811\10666811j.str

chain nodes : 9 11 12 14 16 17 19 18 ring nodes : 25 26 27 1 2 3 4 5 22 23 24 34 35 6-11 11-12 11-14 12-17 12-23 16-17 17-18 18-19 30-31 31-36 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 34-35

34-38 35-36 36-37 37-38

exact/norm bonds :

6-11 11-12 11-14 12-17 12-23 16-17 17-18 18-19 22-23 22-27 23-24 24-25

25-26 26-27 30-31 31-36 34-35 34-38 35-36 36-37 37-38

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2:Ak,H

G3:C,N

G4:H,Cy,Ak

G5:0,S,C

Hydrogen count :
11:>= minimum 1

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS

12:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 22:Atom 23:Atom

24:Atom 25:Atom 26:Atom 27:Atom 30:CLASS 31:CLASS 33:CLASS 34:Atom 35:Atom

36:Atom 37:Atom 38:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 15:16:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 331 TO ITERATE

100.0% PROCESSED 331 ITERATIONS 1 ANSWERS

60 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5529 TO 7711
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 15:16:25 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6833 TO ITERATE

100.0% PROCESSED 6833 ITERATIONS

SEARCH TIME: 00.00.01

L3 60 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 161.33 161.75

FILE 'CAPLUS' ENTERED AT 15:16:30 ON 16 SEP 2005
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FILE COVERS 1907 - 16 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 15 Sep 2005 (20050915/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3 L4 2 L3

=> d ibib abs 1-2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2004:267292 CAPLUS DOCUMENT NUMBER: 140:287259 140:287259
Preparation of amide and sulfonamide ligands for the estrogen receptor
O'Keefe Cameron, Kimberly, Chesworth, Richard Pfizer Products Inc., USA PCT Int. Appl., 143 pp.
CODEN: PIXXO2
Patent TITLE: INVENTOR (S) . PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE

OTHER SOURCE(S): MARPAT 140:287259

The present invention provides amides and sulfonamides (shown as I; variables defined below; many of the examples contain the pyrrolidine ring, e.g. II) that are estrogen receptor (ER) ligands (no data), the pharmaceutically acceptable salts, stereoisomers, and prodrugs thereof,

11

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2001:833284 CAPLUS DOCUMENT NUMBER: 135:371641

Preparation of arylheterocyclylamides as motilin

Preparation of aryineterocyclylamides antagonists
Johnson, Sigmond G.; Rivero, Ralph A.
Ortho-McNeil Pharmaceutical, Inc., USA
PCT Int. Appl., 132 pp.
CODEN: PIXXD2 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

Patent English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

OTHER SOURCE(S):

PATENT NO. KIND DATE APPLICATION NO. DATE A2 A3 20011115 WO 2001085694 WO 2001085694 WO 2001-US11821 20010411 A2 20011115 W0 2001-US11821 20010411
A3 20020404
AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GE, GH, GH, FH, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, IT, MD, MG, MK, MN, MM, MZ, NO, NZ, PL, PT, RO, RU, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, TU, ALS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, FI, FR, GB, GR, IE, IT, LU, MC, ML, FT, SE, TR, BF, CI, CY, GA, GN, GW, ML, MR, ME, SN, TD, TE
2 200310128 AA 20011115 CA 2001-2408288 20010411
A2 2003026 EP 2001-929767 20010410
BC, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, FT, LV, FT, RO, MK, CY, AL, TR
TZ 20031015 JP 2001-582295 20010411
A 20031030 US 2002-291133 20021108
A1 20031030 US 2002-291133 20021108
A1 20031030 US 2002-291133 20011061
A 20031030 US 2002-291133 20011061
BC 2005025 US 2000-020131F US 200106055 VS 20010-291133 A1 20010410
BC 2001-US11821 US 2001-0511821 US 2001-0511821 US 2001-021131821 US 20011091
BARPAT 135:371641 WO 2001085693
WO 2001085693
W: AE, AG, AL,
CR, CU, CZ,
HU, ID, IL,
LU, LV, MA,
SD, SE, SG,
ZA, ZW, AM,
RW: GH, GM, KE,
DE, DK, ES,
BJ, CT, CG,
US 2002013352
US 6511980
CA 2408288
EP 1294695
R: AT, BE, CH,
IE, SI, LT,
JP 2003532710
BG 107243
US 2003203906
US 2005148584
PRIORITY APPLM. INFO:: 20020404

MARPAT 135:371641

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) and the pharmaceutically acceptable salts of the prodrugs. The invention further provides pharmaceutical compns. comprising I, and methods for treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER (e.g. female sexual dyvinction, postmenopausal syndrome, osteoporosis, elevated serum cholesterol levels, and breast or uterine cancer) which comprise administering to a mammalian subject in need of treatment therevith, an effective ant. of I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutical compns. Comprising I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug. The invention further provides pharmaceutical compns. comprising combinations of I and 21 of NaF, estrogen, a bone anabolic agent, a growth hormone or growth hormone secretagogue, a prostaglandin agonist/antagonist, and a parathycoid hormone, and methods of treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER comprising the administration of an effective ant. of such combination to a nammalian subject in need of treatment therevith. Although the methods of prepn. are not claimed, 212 example prepns. are included. For example, II was prepd. in 41% yield by base hydrolysis of its p-toluenesulfonic acid ester, which in turn was prepd. N-acylation of toluene-4-sulfonic acid 4-[[(4-[2-(pyrrolidin-1-yl)ethoxy)phenyl]amino]methyl]phenyl ester by cyclohexanecarbonyl chloride. Toluen-4-sulfonic acid 4-[([4-[2-(pyrrolidin-1-yl)ethoxy)phenyl]mino]methyl]phenyl ester by cyclohexanecarbonyl chloride. Toluen-4-sulfonic acid 4-[(4-[2-(pyrrolidin-1-yl)ethoxy)phenyl]mino]methyl]phenyl ester was prepd. in 2 steps (71 and 801, resp., yields) starting with tosylate formation from 4-hydroxybenzaldehyde followed by imine formation with [4-[2-(pyrrolidin-1-yl-hoxy)phenyl]mino]methyl]phenyl

THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

(Continued) L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

X4R3

R2X1NR1X2AX3

Title compds. [I, Rl = H, (substituted) aryl, aralkyl, heterocyclyl, diarylalkyl, alkyl, etc., R2 = (substituted) aryl, aralkyl, cycloalkyl, heterocyclylalkyl, etc., N1-X4 = null, C0, SO2; RINR2X1 = (substituted) heterocyclyll, A = (substituted) alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, etc., Y = 0, NH, S, SO2; n = 0-5; R4 = H, amino, alkylamino, dialkylamino, heterocyclyl, alkylheterocyclyl, etc.], were prepared Thus, N-[3-[2-(1-pyrrolidinolethoxylphenyl]-N-(cis-3-aminocyclohexyl)methyl-4-fluorophenylcarboxamide (preparation given) and

on PhMe were treated sequentially with Ti(OiPr)4, EtOH, and NaBH(OAc)3 to give a crude residue which in CHZC12 was treated with Me3CCCC1 to give title compound (II). II inhibited motilin-induced contraction in rabbit colon with ICSO = 0.029 µM.

has close shudward and but does not head on amended at his A

STRUCTURE FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9 DICTIONARY FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10666811\10666811i.str

chain nodes : 9 11 12 14 16 17 18 19 30 31 ring nodes : 1 2 3 4 5 6 22 25 26 27 23 24 chain bonds : 6-11 11-12 11-14 12-17 12-23 16-17 17-18 17-43 18-19 ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 22-23 \quad 22-27 \quad 23-24 \quad 24-25 \quad 25-26 \quad 26-27 \quad 34-35$

34-38 35-36 36-37 37-38

exact/norm bonds :

6-11 11-12 11-14 12-17 12-23 16-17 17-18 17-43 18-19 22-23 22-27 23-24

24-25 25-26 26-27 30-31 31-36 34-35 34-38 35-36 36-37 37-38

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2:Ak,H

G3:C,N

G4:H,Cy,Ak

G5:0,S,C

Hydrogen count :

11:>= minimum 1

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 9:CLASS 10:CLASS 11:CLASS

12:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 22:Atom 23:Atom

24:Atom 25:Atom 26:Atom 27:Atom 30:CLASS 31:CLASS 33:CLASS 34:Atom 35:Atom

36:Atom 37:Atom 38:Atom 43:CLASS

L1 STRUCTURE UPLOADED

=> s L1

SAMPLE SEARCH INITIATED 15:12:15 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 71 TO ITERATE

100.0% PROCESSED 71 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 915 TO 1925 PROJECTED ANSWERS: 22 TO 418

L2 11 SEA SSS SAM L1

=> s L1 full

FULL SEARCH INITIATED 15:12:22 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1380 TO ITERATE

100.0% PROCESSED 1380 ITERATIONS 191 ANSWERS

SEARCH TIME: 00.00.02

L3 191 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

11 ANSWERS

FULL ESTIMATED COST 161.33 161.75

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FILE COVERS 1907 - 16 Sep 2005 VOL 143 ISS 13 FILE LAST UPDATED: 15 Sep 2005 (20050915/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3 L4 1 L3

=> d ibib abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
1140:287259
1140:287259
1151:
PATENT ASSIGNEE(S):
PATENT ASSIGNEE(S):
POCUMENT TYPE:
DOCUMENT TYPE:
PANGUAGE:
PANGUAGE:
PANGUAGE:
PANGUAGE:
PANGUAGE:
PANGUAGE:
PATENT INFORMATION:
PATENT INFORMATION:
PATENT INFORMATION:
PATENT INFORMATION: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.		APPLICATION NO.	
		1 WO 2003-IB3824	
		, BA, BB, BG, BR, BY,	
co, cr, cr	, CZ, DE, DK, DF	, DZ, EC, EE, ES, FI,	GB, GD, GE, GH,
GM, HR, HU	, ID, IL, IN, IS	, JP, KE, KG, KP, KR,	KZ, LC, LK, LR,
LS, LT, LU	, LV, MA, MD, MG	, MK, MN, MW, MX, MZ,	NI, NO, NZ, OM,
PH, PL, PT	, RO, RU, SC, SI	, SE, SG, SK, SL, TJ,	TM, TN, TR, TT,
TZ, UA, UG	, US, UZ, VC, VN	I, YU, ZA, ZM, ZW	
RV: GH, GM, KE	, LS, MW, MZ, SC	, SL, SZ, TZ, UG, ZM,	ZW, AM, AZ, BY,
KG, KZ, MI	, RU, TJ, TM, AT	, BE, BG, CH, CY, CZ,	DE, DK, EE, ES,
FI, FR, GE	, GR, HU, IE, IT	, LU, MC, NL, PT, RO,	SE, SI, SK, TR,
BF, BJ, CF	, CG, CI, CM, GA	, GN, GQ, GW, ML, MR,	NE, SN, TD, TG
CA 2499490	AA 2004040	1 CA 2003-2499490	20030908
EP 1542967	A1 2005062	2 EP 2003-797427	20030908
R: AT, BE, CH	, DE, DK, ES, FF	, GB, GR, IT, LI, LU,	NL, SE, MC, PT,
IE, SI, LT	, LV, FI, RO, MP	C, CY, AL, TR, BG, CZ,	EE, HU, SK
		BR 2003-14126	
US 2004110767	A1 2004061	0 US 2003-666811	20030917
PRIORITY APPLN. INFO.:		US 2002-412338P	P 20020920
		WO 2003-IB3824	W 20030908
OTHER SOURCE(S):	MARPAT 140:207	259	

. .1

The present invention provides amides and sulfonamides (shown as I; variables defined below; many of the examples contain the pyrrolidine ring, e.g. II) that are estrogen receptor (ER) ligands (no data), the pharmaceutically acceptable salts, stereoisomers, and prodrugs thereof, AB

II

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) and the pharmaceutically acceptable salts of the prodrugs. The invention further provides pharmaceutical compns. comprising I, and methods for treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER (e.g. female sexual dysfunction, postmenopausal syndrome, osteoporosis, elevated serum cholesterol levels, and breast or uterine cancer) which comprise administering to a mammalian subject in need of treatment therewith, an effective amt. of I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutically acceptable salt of the prodrug. The invention further provides pharmaceutical compns. comprising combinations of I and 21 of NaF, estrogen, a bone anabolic agent, a growth hormone or growth hormone secretagogue, a prostaglandin agonist/antagonist, and a parathycoid hormone, and methods of treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER comprising the administration of an effective amt. of such combination to a mammalian subject in need of treatment therewith. Although the methods of prepn. are not claimed, 212 example prepns, are included. For example, II was prepd. In administration of an effective amt. of such combination to a mammalian subject in need of treatment therewith. Although the methods of prepn. are not claimed, 212 example prepns, are included. For example, II was prepd. In a supple prepn. The production of the production of a method of the production of the productio